

**AMENDMENTS TO THE CLAIMS**

This is a complete and current listing of the claims, marked with status identifiers in parentheses. The following listing of claims will replace all prior versions and listings of claims in the application.

1. (Currently Amended) A method for sampling a state space of a system with states  $x$  and a probability density  $\rho(x)$  indicating the probability for the system to be in state  $x$  by iteratively generating states  $x_{i,t}$  and their weighting factors  $\tilde{\rho}_{i,t}$ , wherein the index  $i$  is the iteration parameter and the index  $t$  distinguishes different states  $x_{i,t}$  generated by an iteration  $i$ , the method comprising:  
sampling the state space of the system and performing,  
a first step for selecting an initial sampling distribution function  $\rho_1(x)$ ,  
a fifth step for performing an analysis and an iteration procedure including  
a second step for generating  $N_j$  states  $x_{j,t}$  by a numerical sampling algorithm and  
a fourth step for testing at least one criterion to decide whether to continue the iteration procedure or to stop the iteration procedure and to go to a fifth step in order to perform the analysis using ~~[[the]]~~ simulated data, wherein the iteration procedure further includes  
a third step determining weighting factors  $\tilde{\rho}_{i,t}$  for states  $x_{i,t}$  generated so far by using sampling distribution functions  $\rho_i(x)$  determined so far, and  
a fitting step for determining a sampling distribution function  $\rho_j(x)$  for the next iteration by fitting  $\rho_j(x)$  to  $\tilde{\rho}_{i,t} \mathcal{O}(x_{i,t})$  for states  $x_{i,t}$

generated so far, wherein  $O(x_{i,t})$  is a function, respectively a property, of the states  $x_{i,t}$ , and  
identifying a desired property in the state space of the system based on sampled state space.

2. (Previously Presented) Method as claimed in claim 1, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is fitted such that it maximizes an objective function preferably defined as a function of local comparisons between the sampling distribution function and the product  $\tilde{\rho}_{i,t}O(x_{i,t})$ .
3. (Previously Presented) Method as claimed in claim 1, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is fitted such that the sampling distribution function  $\rho_j(x)$  is large for at least one state  $x_{i,t}$  with a large product  $\tilde{\rho}_{i,t}O(x_{i,t})$ , and tends to be small for states with a small product  $\tilde{\rho}_{i,t}O(x_{i,t})$ .
4. (Previously Presented) Method as claimed in claim 1, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is a function with at least one constraint.
5. (Previously Presented) Method as claimed in claim 4, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is the distribution function of the system with constraints or a multicanonical distribution function with

constraints.

6. (Previously Presented) Method as claimed in claim 1, wherein the numerical sampling algorithm of at least one iteration generates correlated states  $x_{j,t}$ .
7. (Previously Presented) Method as claimed in claim 4, wherein the fitting of  $\rho_j(x)$  is done by selecting states  $x_{i,t}$  for which the product  $\tilde{\rho}_{i,t}O(x_{i,t})$  has extreme values and by using the selected states  $x_{i,t}$  to define the region in which  $\rho_j(x)$  has extreme values.
8. (Previously Presented) Method as claimed in claim 1, wherein parameters of the sampling distribution function  $\rho_j(x)$  of at least one iteration are determined by a linear least square fit of the logarithm of the un-normalized sampling distribution function  $\rho_j(x)$  to the logarithm of the product  $\tilde{\rho}_{i,t}O(x_{i,t})$ .
9. (Previously Presented) Method as claimed in claim 1, wherein the normalization constant of the sampling distribution function  $\rho_j(x)$  of at least one iteration is estimated from the sampled states  $x_{i,t}$  and their weighting factors  $\tilde{\rho}_{i,t}$ .
10. (Previously Presented) Method as claimed in claim 1, wherein at least three iterations are done.
11. (Previously Presented) Method as claimed in claim 1, wherein the function  $O(x)$  is a function of a set of at least two functions  $\Theta=\{O_1(x), O_2(x), \dots, O_{N_{prep}}(x)\}$ .

12. (Currently Amended) A computer ~~software product~~readable storage  
medium encoded with a computer program including instructions for sampling  
a state space by iteratively generating states  $x_{i,t}$  and their weighting factors  $\tilde{\rho}_{i,t}$ ,  
wherein the index  $i$  is the iteration parameter and the index  $t$  distinguishes  
different states  $x_{i,t}$  generated by an iteration  $i$ , ~~said product including a~~  
~~computer-readable medium in which program instructions are stored, which~~  
instructions, when read by a computer, enable the computer to:  
select an initial sampling distribution function  $\rho(x)$ ,  
to execute a fifth step for performing an analysis,  
and to execute an iteration procedure including,  
a second step for generating  $N_j$  states  $x_{j,t}$  by a numerical sampling algorithm  
and  
a fourth step for testing at least one criterion to decide whether to continue the  
iteration procedure or to stop the iteration procedure and to go to a fifth step in  
order to perform the analysis using the simulated data, wherein the iteration  
further includes  
a third step determining weighting factors  $\tilde{\rho}_{i,t}$  for states  $x_{i,t}$  generated so far by  
using sampling distribution functions  $\rho_i(x)$  determined so far and  
a fitting step for determining a sampling distribution function  $\rho_j(x)$  for the next  
iteration by fitting  $\rho_j(x)$  to  $\tilde{\rho}_{i,t}\alpha(x_{i,t})$  for states  $x_{i,t}$  generated so far, wherein  
 $\alpha(x_{i,t})$  is a function, respectively a property, of the states  $x_{i,t}$ .

13. (Previously Presented) Method as claimed in claim 2, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is fitted such that the sampling distribution function  $\rho_j(x)$  is large for at least one state  $x_{i,t}$  with a large product  $\tilde{\rho}_{i,t}O(x_{i,t})$ , and tends to be small for states with a small product  $\tilde{\rho}_{i,t}O(x_{i,t})$ .
14. (Previously Presented) Method as claimed in claim 1, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is a function with at least one constraint, having an extreme value in the region of at least one selected state  $x_{j,constr}$  and having vanishing values at a distance from the at least one selected state  $x_{j,constr}$ .
15. (Previously Presented) Method as claimed in claim 1, wherein the sampling distribution function  $\rho_j(x)$  of at least one iteration is a function with at least one constraint, having an extreme value in the region of at least one selected state  $x_{j,constr}$  and having vanishing values at a distance from the at least one selected state  $x_{j,constr}$ , wherein the constraint is a harmonic constraint with at least one constant  $k_{constr}$  defining the strength of the constraint at the selected state  $x_{j,constr}$ .
16. (Previously Presented) Method as claimed in claim 1, wherein the numerical sampling algorithm of at least one iteration generates correlated states  $x_{j,t}$ , wherein the sampling distribution function  $\rho_j(x)$  has a maximum that biases sampling into a sub-region of the state space, wherein the sampling distribution

function  $\rho_j(x)$  is fitted such that the maximum is in a region where the product  $\tilde{\rho}_{i,i}O(x_{i,i})$  has a maximum, and wherein the sampling starts from a state close to the maximum of the sampling distribution function  $\rho_j(x)$ .

17. (Previously Presented) Method as claimed in claim 1, wherein the function  $O(x)$  is a function of a set of at least two functions  $\Theta=\{O_1(x), O_2(x), \dots, O_{N_{prop}}(x)\}$ , including at least one of the following functions:
  - at least one property for which at least one estimate is derived in the analysis of the fifth step,
  - at least one function that is large for states that must be sampled to ensure transitions between important regions,
  - the inverse of the probability distribution function of at least one property of the system, and
  - the inverse of the probability distribution of the negative logarithm of the distribution function of the system.
18. (Previously Presented) A computer-readable medium comprising executable program instructions configured to cause a computer to perform the method of claim 1.
19. (Previously Presented) A computer program, adapted to cause a computer to perform the method of claim 1.
20. (Previously Presented) A computer-readable medium comprising the computer program of claim 19.